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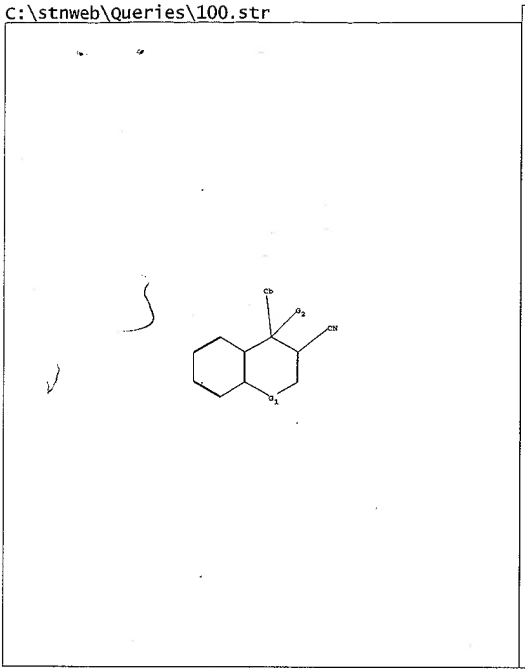

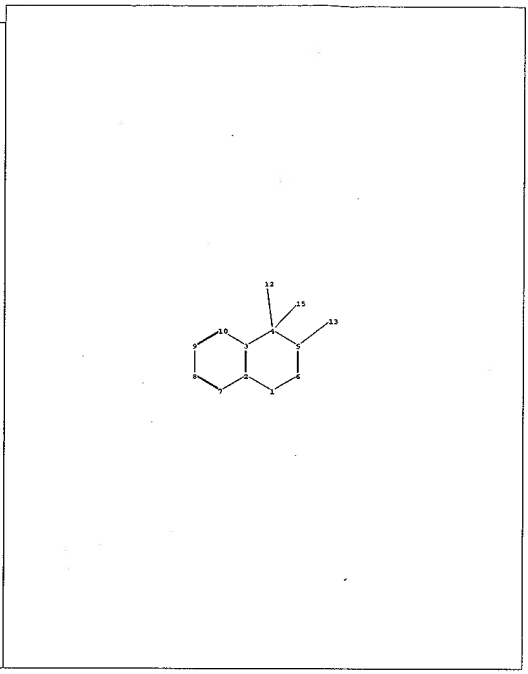

chain nodes :
12 13 15
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
4-12 4-15 5-13
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10
exact/norm bonds :
1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13
normalized bonds :
2-3 2-7 3-10 7-8 8-9 9-10

G1:O,S

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS

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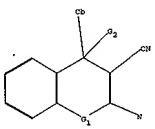

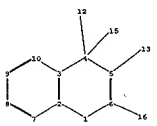

chain nodes :
12 13 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
4-12 4-15 5-13 6-16
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10
exact/norm bonds :
1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13 6-16
normalized bonds :
2-3 2-7 3-10 7-8 8-9 9-10

G1:O,S

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS 16:CLASS

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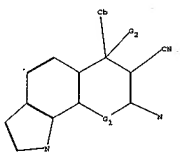

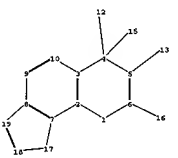

chain nodes :
12 13 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10 17 18 19
chain bonds :
4-12 4-15 5-13 6-16
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 7-17 8-9 8-19 9-10 17-18 18-19
exact/norm bonds :
1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13 6-16 7-17 8-19 17-18 18-19
normalized bonds :
2-3 2-7 3-10 7-8 8-9 9-10
isolated ring systems :
containing 1 :

G1:O,S

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom

```
* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

NEWS  1              Web Page URLs for STN Seminar Schedule - N. America
NEWS  2              "Ask CAS" for self-help around the clock
NEWS  3   SEP 09     CA/CAplus records now contain indexing from 1907 to the
                     present
NEWS  4   AUG 05     New pricing for EUROPATFULL and PCTFULL effective
                     August 1, 2003
NEWS  5   AUG 13     Field Availability (/FA) field enhanced in BEILSTEIN
NEWS  6   AUG 18     Data available for download as a PDF in RDISCLOSURE
NEWS  7   AUG 18     Simultaneous left and right truncation added to PASCAL
NEWS  8   AUG 18     FROSTI and KOSMET enhanced with Simultaneous Left and Righ
                     Truncation
NEWS  9   AUG 18     Simultaneous left and right truncation added to ANABSTR
NEWS 10   SEP 22     DIPPR file reloaded
NEWS 11   DEC 08     INPADOC: Legal Status data reloaded
NEWS 12   SEP 29     DISSABS now available on STN
NEWS 13   OCT 10     PCTFULL: Two new display fields added
NEWS 14   OCT 21     BIOSIS file reloaded and enhanced
NEWS 15   OCT 28     BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16   NOV 24     MSDS-CCOHS file reloaded
NEWS 17   DEC 08     CABA reloaded with left truncation
NEWS 18   DEC 08     IMS file names changed
NEWS 19   DEC 09     Experimental property data collected by CAS now available
                     in REGISTRY
NEWS 20   DEC 09     STN Entry Date available for display in REGISTRY and CA/CAplus

NEWS EXPRESS  NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:01:27 ON 12 DEC 2003

=> filereg
FILEREG IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    0.21        0.21
```

FILE 'REGISTRY' ENTERED AT 11:01:37 ON 12 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0
DICTIONARY FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

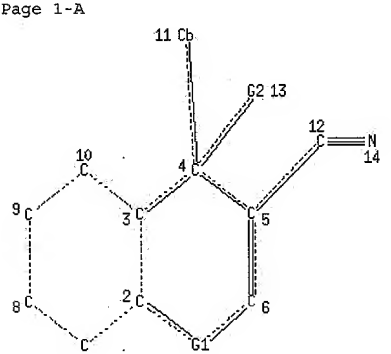
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

H 17 Ak 18

O 15 S 16
Page 1-A



Page 1-B

7 1
Page 2-B
VAR G1=15/16
VAR G2=17/18
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3

```
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS R      AT  10
NSPEC   IS C      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  12 14 17 18
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 11:06:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    574 TO ITERATE

100.0% PROCESSED     574 ITERATIONS                          49 ANSWERS
SEARCH TIME: 00.00.01

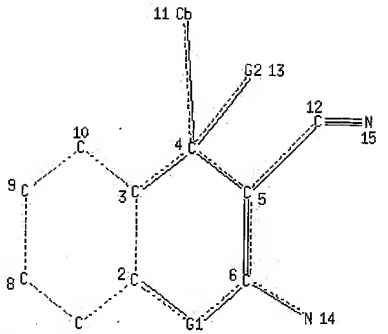
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        10043 TO    12917
PROJECTED ANSWERS:             560 TO     1400

L2            49 SEA SSS SAM L1

=>
L3       STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3                STR
 H 18 Ak 19

 0 16 S 17
Page 1-A
```



Page 1-B

7 1

Page 2-B

VAR G1=16/17
VAR G2=18/19
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS C AT 11
NSPEC IS C AT 12
NSPEC IS C AT 13
NSPEC IS C AT 14
NSPEC IS C AT 15
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 12 14 15 18 19
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

=> s 13
SAMPLE SEARCH INITIATED 11:07:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 298 TO ITERATE

100.0% PROCESSED 298 ITERATIONS 49 ANSWERS
SEARCH TIME: 00.00.01

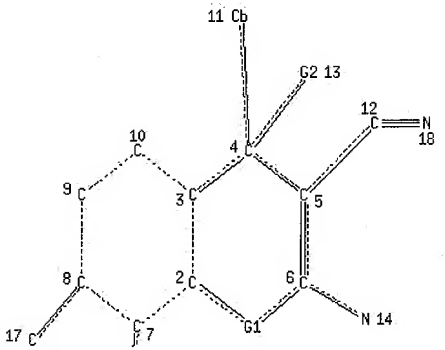
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4925 TO 6995
PROJECTED ANSWERS: 560 TO 1400

```
L4             49 SEA SSS SAM L3

=>
L5       STRUCTURE UPLOADED

=> d 15
L5 HAS NO ANSWERS
L5                 STR
 H 21 Ak 22

 0 19 S 20
Page 1-A
```

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Page 1-B
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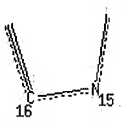


```
Page 2-B
VAR G1=19/20
VAR G2=21/22
NODE ATTRIBUTES:
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS R       AT   7
NSPEC    IS R       AT   8
NSPEC    IS R       AT   9
NSPEC    IS R       AT  10
NSPEC    IS C       AT  11
NSPEC    IS C       AT  12
NSPEC    IS C       AT  13
NSPEC    IS C       AT  14
NSPEC    IS R       AT  15
NSPEC    IS R       AT  16
NSPEC    IS R       AT  17
```

```
NSPEC   IS C      AT  18
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  12 14 18 21 22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE


=> s l5
SAMPLE SEARCH INITIATED 11:08:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      4 TO ITERATE

100.0% PROCESSED       4 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            4 TO       200
PROJECTED ANSWERS:               0 TO         0

L6            0 SEA SSS SAM L5

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 11:08:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     115 TO ITERATE

100.0% PROCESSED     115 ITERATIONS                             10 ANSWERS
SEARCH TIME: 00.00.01

L7           10 SEA SSS FUL L5

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE       TOTAL
                                                 ENTRY     SESSION
FULL ESTIMATED COST                             152.55      152.76

FILE 'HCAPLUS' ENTERED AT 11:08:36 ON 12 DEC 2003
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FILE COVERS 1907 - 12 Dec 2003  VOL 139 ISS 25
FILE LAST UPDATED: 11 Dec 2003  (20031211/ED)
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 1 L7

=> d l8, ibib abs fhitstr, 1

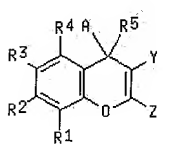
L8 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:888735 HCAPLUS
DOCUMENT NUMBER: 137:369971
TITLE: Preparation of substituted 4H-chromenes and analogs as activators of caspases and inducers of apoptosis and their uses against cancer and other disorders
INVENTOR(S): Cai, Sui Xiong; Zhang, Hong; Jiang, Songchun; Storer, Richard
PATENT ASSIGNEE(S): Cytovia, Inc., USA
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092594	A1	20021121	WO 2002-US15399	20020516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003065018	A1	20030403	US 2002-146138	20020516

PRIORITY APPLN. INFO.: US 2001-290997P P 20010516
OTHER SOURCE(S): MARPAT 137:369971
GI



I

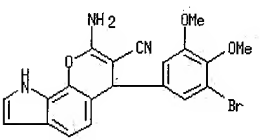
AB The present invention is directed to substituted 4H-chromenes and analogs thereof (shown as I; e.g. 2-amino-3-cyano-7-hydroxy-4-(3-bromo-4,5-dimethoxyphenyl)-4H-chromene). It also relates to the discovery that I are activators of caspases and inducers of apoptosis and, therefore, can be used to induce cell death in a variety of clin. conditions in which controlled growth and spread of abnormal cells occurs. In I: R1-R4 = H,

halo, haloalkyl, aryl, fused aryl, carbocyclic, heterocyclic, heteroaryl, C1-10 alkyl, alkenyl, alkynyl, arylalkyl, arylalkenyl, arylalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl, aminoalkyl, carboxyalkyl, nitro, amino, cyano, acylamido, hydroxy, thiol, acyloxy, azido, alkoxy, carboxy, methylenedioxy, carbonylamido or alkylthio; or R1 and R2, or R2 and R3, or R3 and R4, taken together with the atoms to which they are attached form an aryl, heteroaryl, partially satd. carbocyclic or partially satd. heterocyclic group, wherein said group is optionally substituted. R5 is H or C1-10 alkyl; A is optionally substituted and is aryl, heteroaryl, satd. carbocyclic, partially satd. carbocyclic, satd. heterocyclic, partially satd. heterocyclic or arylalkyl; Y is CN, COR7, CO2R7 or CONRxRy, wherein R7, Rx and Ry = H, C1-10 alkyl, haloalkyl, aryl, fused aryl, carbocyclic, heterocyclic, heteroaryl, alkenyl, alkynyl, arylalkyl, arylalkenyl, arylalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl or aminoalkyl; or Rx and Ry are taken together with the N to which they are attached to form a heterocycle; and Z is NR8R9, NHCOR8, N(COR9)2, N(COR8)(COR9), N:CHOR8 or N:CHR8, wherein R8 and R9 = H, C1-4 alkyl or aryl, or R8 and R9 are combined together with the group attached to them to form a heterocycle. The EC50 values for >80 I against T-47D and ZR-75-1 human breast cancer cell lines are tabulated, e.g. 30 and 25 nM, resp., for 2-amino-3-cyano-4-(3-bromo-4,5-dimethoxyphenyl)-4H-indolo[7,6-b]pyran. Although the methods of prepn. are not claimed, 81 example prepns. are included.

IT **475576-80-8P**, 2-Amino-3-cyano-4-(3-bromo-4,5-dimethoxyphenyl)-4H-indolo[7,6-b]pyran
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of substituted 4H-chromenes and analogs as activators of caspases and inducers of apoptosis and their uses against cancer and other disorders)

RN 475576-80-8 HCAPLUS

CN Pyrano[3,2-g]indole-3-carbonitrile, 2-amino-4-(3-bromo-4,5-dimethoxyphenyl)-4,9-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.79	159.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

FILE 'CAOLD' ENTERED AT 11:08:48 ON 12 DEC 2003
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=>  d his

     (FILE 'HOME' ENTERED AT 11:01:27 ON 12 DEC 2003)

     FILE 'REGISTRY' ENTERED AT 11:01:37 ON 12 DEC 2003
L1              STRUCTURE UPLOADED
L2           49 S L1
L3              STRUCTURE UPLOADED
L4           49 S L3
L5              STRUCTURE UPLOADED
L6            0 S L5
L7           10 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 11:08:36 ON 12 DEC 2003
L8            1 S L7

     FILE 'CAOLD' ENTERED AT 11:08:48 ON 12 DEC 2003

=> s l7
L9            0 L7

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.40     159.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -0.65

STN INTERNATIONAL LOGOFF AT 11:08:56 ON 12 DEC 2003
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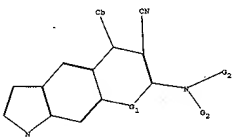
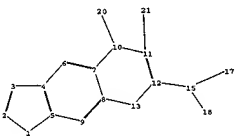




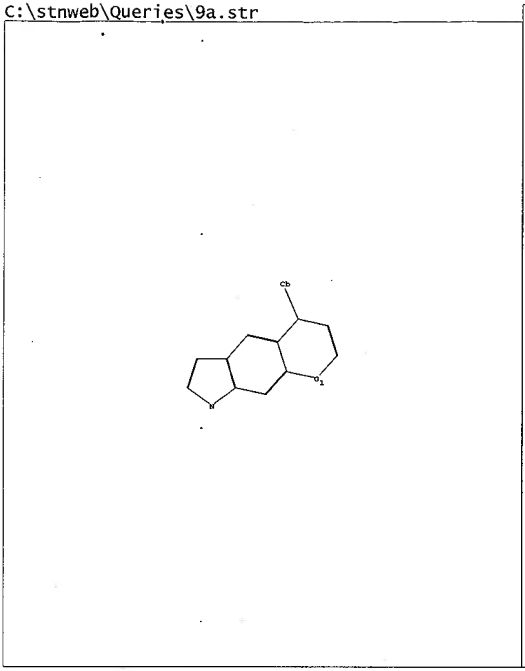
chain nodes :
15 17 18 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
10-20 11-21 12-15 15-17 15-18
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13
exact/norm bonds :
1-2 1-5 2-3 3-4 7-10 8-13 10-11 10-20 11-12 11-21 12-13 12-15 15-17 15-18
normalized bonds :
4-5 4-6 5-9 6-7 7-8 8-9

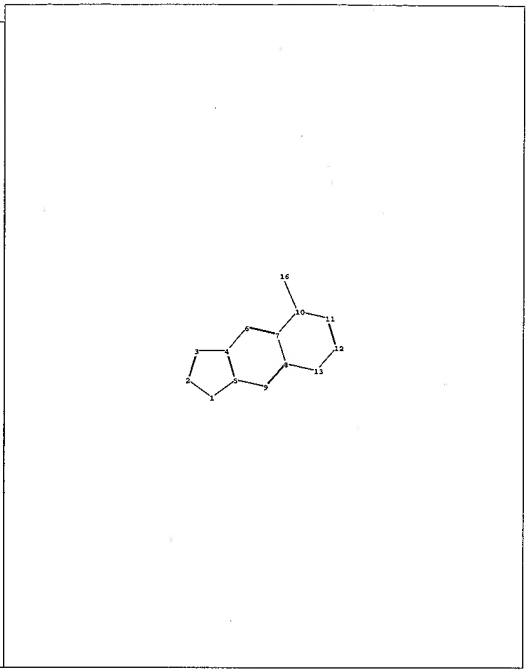
G1:O,S

G2:Ak,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 15:CLASS 17:CLASS 18:CLASS 20:Atom 21:CLASS

C:\stnweb\Queries\9a.str





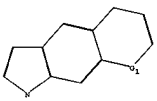
chain nodes :
16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
10-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13
exact/norm bonds :
1-2 1-5 2-3 3-4 7-10 8-13 10-11 10-16 11-12 12-13
normalized bonds :
4-5 4-6 5-9 6-7 7-8 8-9

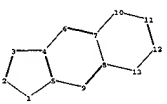
G1:O,S

G2:Ak,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 16:Atom

C:\stnweb\Queries\9b.str





ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13
exact/norm bonds :
1-2 1-5 2-3 3-4 7-10 8-13 10-11 11-12 12-13
normalized bonds :
4-5 4-6 5-9 6-7 7-8 8-9

G1:O,S

G2:Ak,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom

```
* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
NEWS  2            "Ask CAS" for self-help around the clock
NEWS  3  SEP 09    CA/CAplus records now contain indexing from 1907 to the
                   present
NEWS  4  AUG 05    New pricing for EUROPATFULL and PCTFULL effective
                   August 1, 2003
NEWS  5  AUG 13    Field Availability (/FA) field enhanced in BEILSTEIN
NEWS  6  AUG 18    Data available for download as a PDF in RDISCLOSURE
NEWS  7  AUG 18    Simultaneous left and right truncation added to PASCAL
NEWS  8  AUG 18    FROSTI and KOSMET enhanced with Simultaneous Left and Righ
                   Truncation
NEWS  9  AUG 18    Simultaneous left and right truncation added to ANABSTR
NEWS 10  SEP 22    DIPPR file reloaded
NEWS 11  DEC 08    INPADOC: Legal Status data reloaded
NEWS 12  SEP 29    DISSABS now available on STN
NEWS 13  OCT 10    PCTFULL: Two new display fields added
NEWS 14  OCT 21    BIOSIS file reloaded and enhanced
NEWS 15  OCT 28    BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16  NOV 24    MSDS-CCOHS file reloaded
NEWS 17  DEC 08    CABA reloaded with left truncation
NEWS 18  DEC 08    IMS file names changed
NEWS 19  DEC 09    Experimental property data collected by CAS now available
                   in REGISTRY
NEWS 20  DEC 09    STN Entry Date available for display in REGISTRY and CA/CAplus

NEWS EXPRESS  NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:28:25 ON 12 DEC 2003

=> g
G IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    0.21        0.21
```

FILE 'REGISTRY' ENTERED AT 10:28:33 ON 12 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0
DICTIONARY FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

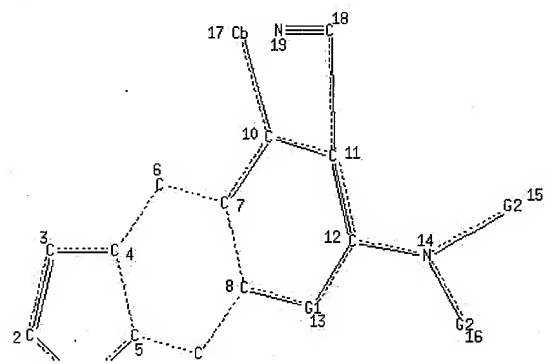
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

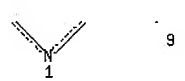
=>
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
Ak 22H 23

0 20 S 21
Page 1-A



Page 1-B



Page 2-B
VAR G1=20/21
VAR G2=22/23

```
NODE ATTRIBUTES:
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS R      AT  10
NSPEC   IS R      AT  11
NSPEC   IS R      AT  12
NSPEC   IS R      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  14 18 19 22 23
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  23

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 10:31:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     42 TO ITERATE

100.0% PROCESSED      42 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          452 TO     1228
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:31:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    997 TO ITERATE

100.0% PROCESSED     997 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

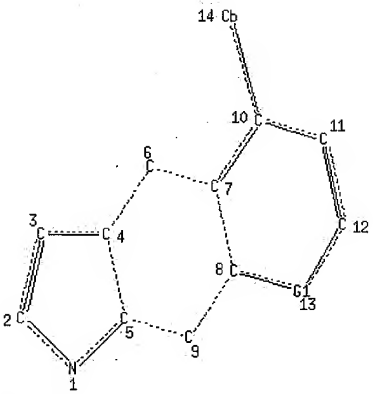
L3            0 SEA SSS FUL L1

=>
L4      STRUCTURE UPLOADED

=> d l4
```

L4 HAS NO ANSWERS
L4 STR

0 15 S 16
Page 1-A



Page 1-B
VAR G1=15/16
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS R AT 11
NSPEC IS R AT 12
NSPEC IS R AT 13
NSPEC IS C AT 14
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

=> s 14
SAMPLE SEARCH INITIATED 10:32:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3002 TO ITERATE

33.3% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

```
                          BATCH    **COMPLETE**
PROJECTED ITERATIONS:          56755 TO     63325
PROJECTED ANSWERS:                 0 TO         0

L5             0 SEA SSS SAM L4

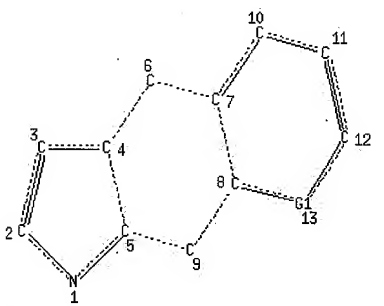
=> s l4 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:32:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  59948 TO ITERATE

100.0% PROCESSED   59948 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L4

=>
L7      STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7                STR
 0 14 S 15
Page 1-A
```




```
Page 1-B
VAR G1=14/15
NODE ATTRIBUTES:
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS R       AT   7
NSPEC    IS R       AT   8
NSPEC    IS R       AT   9
NSPEC    IS R       AT  10
NSPEC    IS R       AT  11
NSPEC    IS R       AT  12
NSPEC    IS R       AT  13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

```
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE


=> s l7
SAMPLE SEARCH INITIATED 10:32:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3002 TO ITERATE

 33.3% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        56755 TO     63325
PROJECTED ANSWERS:               0 TO         0

L8             0 SEA SSS SAM L7

=> s l7 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:32:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  59948 TO ITERATE

100.0% PROCESSED   59948 ITERATIONS                              24 ANSWERS
SEARCH TIME: 00.00.01

L9            24 SEA SSS FUL L7

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             446.05     446.26

FILE 'HCAPLUS' ENTERED AT 10:33:01 ON 12 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 12 Dec 2003  VOL 139 ISS 25
FILE LAST UPDATED: 11 Dec 2003  (20031211/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
```

=> s l9
L10 8 L9

=> d l10, ibib abs fhitstr, 1-8

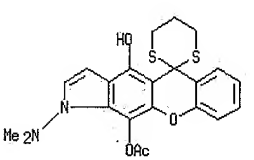
L10 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1996:689416 HCAPLUS
DOCUMENT NUMBER: 126:7949
TITLE: Novel Construction of Highly-Substituted Xanthones
AUTHOR(S): Sun, Lijun; Liebeskind, Lanny S.
CORPORATE SOURCE: Sanford S. Atwood Chemistry Center, Emory University, Atlanta, GA, 30322, USA
SOURCE: Journal of the American Chemical Society (1996), 118(49), 12473-12474
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:7949

AB O-, C-Dianions generated from dithiane protected salicylaldehydes condense with esters of squaric acid in a two-step process to provide γ-benzopyrone-fused cyclobutenediones, with the benzopyrone still protected as the dithiane. These versatile cyclobutenediones undergo regiospecific 1,2-addn. of unsatd. organolithium reagents (Ph, substituted Ph, 1- and 2-naphthyl, 2- and 3-furyl, 2-thienyl, 2-pyrrolyl, 2-indolyl, β-styryl, 2-dihydropyranyl) at the most electrophilic and least hindered cyclobutenedione carbonyl group. The 1,2-adducts rearrange either spontaneously at room temp. or on brief warming in THF soln. to give, after hydrolysis of the dithiane, a wide variety of substituted xanthones and xanthones linearly fused to arom., heteroarom., and heterocyclic rings.

IT **184023-43-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of xanthones)
RN 184023-43-6 HCAPLUS
CN Spiro[[1]benzopyrano[3,2-f]indole-5(1H),2'-[1,3]dithiane]-4,11-diol, 1-(dimethylamino)-, 11-acetate (9CI) (CA INDEX NAME)

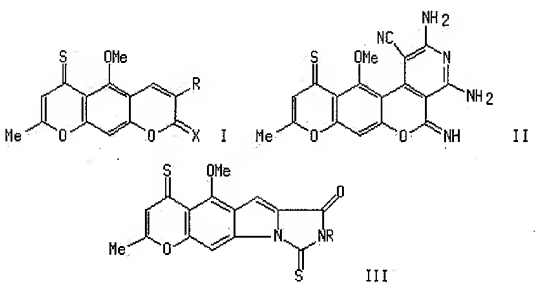


L10 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1991:101768 HCAPLUS
DOCUMENT NUMBER: 114:101768
TITLE: Benzodipyranthione derivatives of expected biological activities
AUTHOR(S): Abdelaziz, Mahfouz A.

CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
SOURCE: Egyptian Journal of Pharmaceutical Sciences (1990), 31(1-4), 561-70
CODEN: EJPSBZ; ISSN: 0301-5068
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



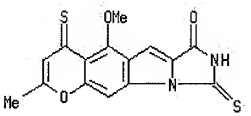
I II III

AB 6-Formyl-7-hydroxy-5-methoxy-2-methylbenzopyran-4-thione reacted with cyanoethanoic acid hydrazide, 2-amino-1,1,3-tricyanoprop-1-ene, benzoylacetonitrile, malononitrile and 2-thiohydantoins to afford heterocycles , e.g., benzodipyrans I [X=O,NH; R = CONHNH2; X=NH, R = C(NH2):C(CN)2; X = O, NH; R = COPh, cyano], pyranobenzopyranopyridine II and benzopyranopyrroloimidazolinethiones III (R = H, Ph).

IT 132369-76-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 132369-76-7 HCAPLUS

CN 4H,7H-Imidazo[1,5-a]pyrano[3,2-f]indol-7-one, 8,9-dihydro-5-methoxy-2-methyl-4,9-dithioxo- (9CI) (CA INDEX NAME)

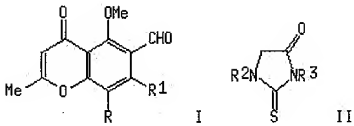


L10 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

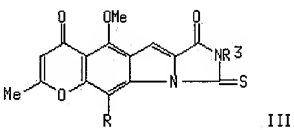
Full Text | Citing References

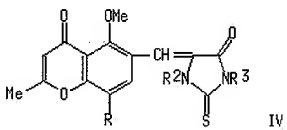
ACCESSION NUMBER: 1990:7422 HCAPLUS
DOCUMENT NUMBER: 112:7422
TITLE: New synthesis of chromonopyrroloimidazolinones and arylidenethioxoimidazolinones. Study of their antimicrobial activities
AUTHOR(S): Aziz, Mahfouz A. Abdel; Riad, Bahia Y.; Shalaby, A. M.
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
SOURCE: Archives of Pharmacal Research (1989), 12(1), 12-16
CODEN: APHRDQ; ISSN: 0253-6269
DOCUMENT TYPE: Journal

LANGUAGE: English
GI


I

II


III

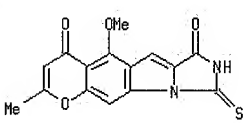

IV

AB 6-Formyl-5-methoxy-2-methylchromone derivs. I (R = H, NO2, Br, R1 = OH; R = H, R1 = OMe) condensed with 2-thioxo-4-imidazolinones II (R2 = H, R3 = H, Ph; R2 = Ph, R3 = H) to form the corresponding chromonopyrroloimidazolinones III or the arylidenethioxoimidazolinones IV. The activity of the imidazole moiety NH of III (R = R3 = H) (V) was confirmed by formation of the Mannich bases. Moreover, alkylation of V was gave alkylmercapto derivs. The antimicrobial activities of compds. II and IV were studied.

IT **124041-37-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and alkylation or Mannich reactions of)

RN 124041-37-8 HCAPLUS

CN 4H,7H-Imidazo[1,5-a]pyrano[3,2-f]indole-4,7-dione, 8,9-dihydro-5-methoxy-2-methyl-9-thioxo- (9CI) (CA INDEX NAME)

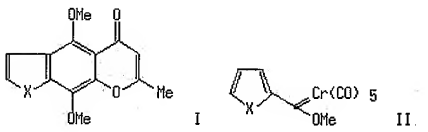


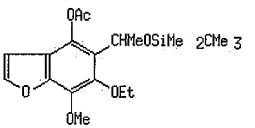
L10 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

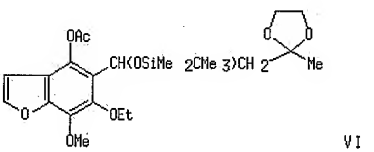
Full Text | Citing References

ACCESSION NUMBER: 1989:457344 HCAPLUS
DOCUMENT NUMBER: 111:57344
TITLE: Synthesis of khellin and its analogs via chromium carbene complexes
AUTHOR(S): Yamashita, A.; Toy, A.; Scahill, T. A.
CORPORATE SOURCE: Res. Lab., Upjohn Co., Kalamazoo, MI, 49001, USA

SOURCE: Journal of Organic Chemistry (1989), 54(15), 3625-34
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:57344
GI



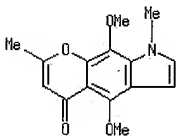




AB The synthesis of khellin (I; X = O), a lipid-altering and antiatherosclerotic furochromone, was accomplished by two different routes in six and seven steps, resp. The key steps in two alternative approaches are the cycloaddn. reactions of a furan-methoxy chromium carbene complex II (X = O) with EtOC≡CCHROSiMe2CMe3 [R = Me (III), 2-methyl-1,3-dioxolan-2-yl (IV)] to provide the direct construction of the benzofuran acetates V and VI, which bear the functional groups necessary for formation of the γ-pyrone ring. The reactions of II (X = O) with alkoxyalkynes in the presence of Ac20 and Et3N in THF provided the acetate derivs. of the desired benzofurans in fair to good yields. The alkoxyalkyne III introduces the acetyl group precursor and IV bears the masked β-diketone unit. The benzofuran acetate V leads to khellinone in four steps by direct conversion of the acetate to a Me ether, the conversion of the silyloxy to the ketone, and the selective cleavage of the Et ether. The other benzofuran acetate VI leads to khellinquinone in five steps by the direct conversion of the acetate to the Me ether, the conversion of the silyloxy ether to a ketone, oxidn. of the p-dimethoxybenzene ring, and sequential aq. acid-catalyzed pyrone ring formation. Khellinone and khellinquinone are converted to I independently by known procedures. These two synthetic routes are applied to the syntheses of khellin analogs, such as the pyrrole (I; X = NMe) and phenyl (I; X = CH:CH) analogs of khellin, using the reactions of the resp. pyrrolyl or Ph chromium carbene complexes II (X = NMe, CH:CH) with III and IV.

IT **121444-68-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

RN 121444-68-6 HCAPLUS
CN Pyrano[3,2-f]indol-4(8H)-one, 5,9-dimethoxy-2,8-dimethyl- (9CI) (CA INDEX NAME)



Z = Me

L10 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

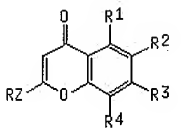
Full Text | Citing References

ACCESSION NUMBER: 1986:68836 HCAPLUS
DOCUMENT NUMBER: 104:68836
TITLE: Benzopyran derivatives and anti-asthma compositions containing them
INVENTOR(S): Gould, Kenneth John; Suschitzky, John Louis; Dicker, Ian Douglas
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Eur. Pat. Appl., 118 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

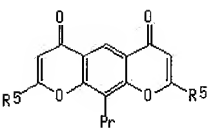
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 150966	A2	19850807	EP 1985-300381	19850121
EP 150966	A3	19860625		
EP 150966	B1	19890712		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 44530	E	19890715	AT 1985-300381	19850121
ZA 8500550	A	19851127	ZA 1985-550	19850123
DK 8500313	A	19850727	DK 1985-313	19850124
DK 162893	B	19911223		
FI 8500324	A	19850727	FI 1985-324	19850125
FI 84482	B	19910830		
FI 84482	C	19911210		
NO 8500303	A	19850729	NO 1985-303	19850125
JP 60163877	A2	19850826	JP 1985-11134	19850125
ES 539846	A1	19870501	ES 1985-539846	19850125
CA 1268460	A1	19900501	CA 1985-472848	19850125
IL 74166	A1	19901105	IL 1985-74166	19850125
US 4670452	A	19870602	US 1985-695459	19850128
US 4698345	A	19871006	US 1985-695460	19850128
AU 8538194	A1	19850801	AU 1985-38194	19850130
AU 582135	B2	19890316		
CA 1250584	A1	19890228	CA 1985-473177	19850130
CN 85105645	A	19870128	CN 1985-105645	19850724
CN 1010855	B	19901219		
ES 554962	A1	19870701	ES 1986-554962	19860514

PRIORITY APPLN. INFO.:
GB 1984-2047 19840126
GB 1984-2577 19840201
EP 1985-300381 19850121

GI



I



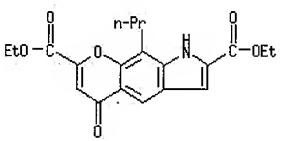
II

AB Antiasthmatic (no data) title compds. [I; R = CO2H, tetrazol-5-yl; adjacent pairs of R1-R4 = atoms required to complete an (un)substituted 5- or 6-membered arom. or heteroarom. ring; Z = bond, (CH2)m, arylene, m = 1-10] were prepd. Thus, di-Et 4,6-dioxo-10-propyl-4H,6H-benzo[1,2-b:5,4-b']dipyran-2,8-dicarboxylate (II, R5 = CO2Et) was treated with NH3 in EtOH to give II (R5 = CONH2) which was dehydrated by heating in DMF with POCl3 to give II (R5 = cyano). This was heated at 60° with NaN3 in DMF to give II (R5 = 1H-tetrazol-5-yl), converted to its di-Na salt.

IT 99370-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sapon. of)

RN 99370-80-6 HCAPLUS

CN Pyrano[3,2-f]indole-2,7-dicarboxylic acid, 4,8-dihydro-4-oxo-9-propyl-, diethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1972:434319 HCAPLUS
DOCUMENT NUMBER: 77:34319
TITLE: Antiinflammatory 2,3-bis(p-methoxyphenyl)indole-5-carboxylic acid derivatives
INVENTOR(S): Szmuszkovicz, Jacob
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: U.S., 8 pp. Division of U.S. 3,565,912 (CA 75;35734t). CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3654308	A	19720404	US 1970-65315	19700819

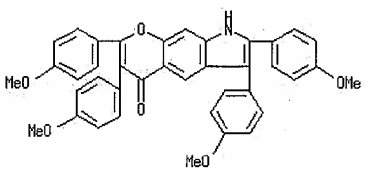
PRIORITY APPLN. INFO.: US 1970-65315 19700819
GI For diagram(s), see printed CA Issue.
AB Division of U.S. 3,565,912 (CA 75: 35734t). Four antiinflammatory 5-alkanoyl-2,3-bis (p-methoxyphenyl)indoles I (R = H, Me; R1 = H, Me, Ac)

were prepd. Anisoin and p-H2NC6H4CO2Et refluxed 2 hr in xylene in the presence of p-MeC6H4SO3H gave 81% Et p-[[p-methoxy-α-(p-methoxyphenyl)phenacyl]amino]benzoate, which on further heating with p-H2NC6H4CO2Et and pMeC6H4SO3H gave II (R = Et, R1 = H). Refluxing II (R = Et, R1 = H) in aq. alc. with KOH gave its corresponding acid, which was then refluxed in C6H6 with SOCl2, and the product added to CdCl2 and MeMgBr in Et2O, refluxed 4 hr to give I (R = Me, R1 = H). Formulations of I were given. The following II (R1 = H) (R = (CH2)2OH, Et, H) were claimed.

IT 23659-79-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 23659-79-2 HCAPLUS

CN Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:435734 HCAPLUS
DOCUMENT NUMBER: 75:35734
TITLE: Antiinflammatory 5-alkanoyl-2,3-bis(p-methoxyphenyl)indoles
INVENTOR(S): Szmuszkovicz, Jacob
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3565912	A	19710223	US 1969-794402	19690127

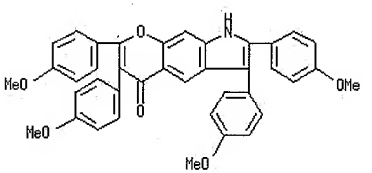
PRIORITY APPLN. INFO.: US 1969-794402 19690127

GI For diagram(s), see printed CA Issue.

AB The title indoles (I, R = H, Me, or Ac; R1 = H, Me, Et, HO, EtO, iso-Pr) are produced by heating p-H2NC6H4CO2R1 with anisoin in the presence of an acid catalyst and further heating with an alkyl p-aminobenzoate and acid catalyst, sapong. the alkyl 2,3-bis(p-methoxyphenyl)indole-5-carboxylate, converting to the acyl chloride and treating the chloride in the presence of CdCl2 with RMgX. The product was treated with NaH and alkyl halide or acyl halide. Alternatively, p-H2NNHC6H4CO2R1 was heated with deoxyanisoin, the mixt. refluxed with alc. HCl or HOCH2CH2OH, and the ester of 2,3-bis(p-methoxyphenyl)-indole-5-carboxylic acid treated to give the free acid, which was then converted as above to I. Thus anisoin and p-H2NC6H4CO2Et refluxed in xylene in the presence of p-MeC6H4SO3H yielded 81% Et p-[[p-methoxy α-(p-methoxyphenyl)phenacyl]-amino benzoate,

which was heated with p-H2NC6H4CO2Et to give I (R = H, R1 = OEt) (II) Et 2,3-bis(p-methoxyphenyl)indole-5-carboxylate. II refluxed in aq. alc with KOH gave I (R = H, R1 = OH) (III), m. 295-7°. Equimolar amts. of p-EtO2CC6H4NHNH2 and deoxyanisoin refluxed with HOCH2CH2OH yielded 2-(hydroxyethyl)-2,3-bis(p-methoxyphenyl)indole-5-carboxylate, which was hydrolyzed and acidified as above to give III. III refluxed in C6H6 with SOCl2 and the product added to CdCl2 and MeMgBr in Et2O and refluxed 4 hr gave I (R = Me, R1 = H) (IV), m. 227-3°.

IT **23659-79-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 23659-79-2 HCAPLUS
CN Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

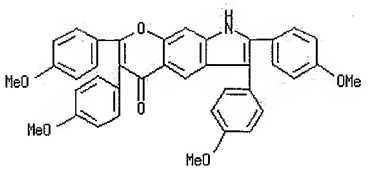
Full Text | Citing References

ACCESSION NUMBER: 1969:491199 HCAPLUS
DOCUMENT NUMBER: 71:91199
TITLE: Synthesis and antiinflammatory activity of 5-substituted 2,3-bis(p-methoxyphenyl)indoles
AUTHOR(S): Youngdale, Gilbert A.; Glenn, E. Myles; Lednicer, Daniel; Szmuszkovicz, Jacob
CORPORATE SOURCE: Res. Lab., Upjohn Co., Kalamazoo, MI, USA
SOURCE: Journal of Medicinal Chemistry (1969), 12, 948-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB p-Carbethoxyphenylhydrazine is treated with deoxyanisoin to give Et 2,3-bis(p-carbethoxyphenyl)indole-5-carboxylate (I), 2,3,6,7-tetrakis(p-carbethoxyphenyl)pyrano-[3,2-f]indolin-4(8H)-one (II) is obtained as a by-product. I is transesterified to give III; IV and V are prepd. from III. The antiinflammatory activity of V is equal to that of VI.

IT **23659-79-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 23659-79-2 HCAPLUS
CN Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

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